di-(1-Methyl-2-methoxybutyl)sebacate

Inchi: InChI=1S/C20H38O6/c1-15(23-5)17(3)25-19(21)13-11-9-7-8-10-12-14-20(22)26-18(4)16
InchiKey: NCGXKOTZQIIEHO-UHFFFAOYSA-N
Formula: C20H38O6
SMILES: COC(C)C(C)OC(=O)CCCCCCCCC(=O)OC(C)C(C)OC
Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-570.08	kJ/mol	Joback Method
hf	-1231.29	kJ/mol	Joback Method
hfus	41.41	kJ/mol	Joback Method
hvap	81.69	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.040		Crippen Method
mcvol	319.280	ml/mol	McGowan Method
pc	1076.39	kPa	Joback Method
rinpol	2188.00		NIST Webbook
tb	852.66	K	Joback Method
tc	1045.73	K	Joback Method
tf	443.94	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.16	J/mol×K	852.66	Joback Method
cpg	1110.51	J/mol×K	1013.56	Joback Method
cpg	1097.85	J/mol×K	981.38	Joback Method
cpg	1083.89	J/mol×K	949.20	Joback Method
cpg	1068.62	J/mol×K	917.02	Joback Method
cpg	1052.04	J/mol×K	884.84	Joback Method
cpg	1121.85	J/mol×K	1045.73	Joback Method
dvisc	0.0000209	Pa×s	852.66	Joback Method
dvisc	0.0000293	Pa×s	784.54	Joback Method

dvisc	0.0000438	Pa×s	716.42	Joback Method
dvisc	0.0000713	Pa×s	648.30	Joback Method
dvisc	0.0001302	Pa×s	580.18	Joback Method
dvisc	0.0002792	Pa×s	512.06	Joback Method
dvisc	0.0007563	Pa×s	443.94	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541874&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume